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Hierarchical nanoreinforced composites: Computational analysis of damage mechanisms

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Abstract. The potential of hierarchical composites with secondary nanoreinforcement is discussed and analysed on the basis of the computational modelling. The concept of nanostructuring of interfaces as an important reserve of the improvement of the composite properties is discussed. The influence of distribution, shape, orientation of nanoparticles (carbon nanotube, graphene) in unidirectional polymer matrix composites on the strength and damage resistance of the composites is studied in computational studies. The possible directions of the improvement of nanoreinforced composites by controlling shapes, localization and other parameters of nanoreinforcements are reviewed.

1. Introduction

Lightweight strong materials are sought for in many areas of industry. Most often, polymer based composites are considered as most promising lightweight strong materials. However, further enhancement of the composite properties is required for many applications, including better lifetime and fatigue resistance, multiple applications, and so on. In order to achieve the enhancement of the composite properties, improvement of constituents (fiber, polymer) and manufacturing technologies is used. The development of hybrid composites, with nanoeingineered phases, is a very promising direction to design lightweight materials with improved properties [1].

The fiber reinforced composites with nanoengineered matrix show often much better performances than the composites without any nanoreinforcements. For instance, 80% improvement of fracture toughness of carbon fiber reinforced epoxy composites achieved as a result of 0.5 wt.% CNT addition of carbon nanotubes (CNTs) [2]. 30% enhancement of the interlaminar shear strength of woven carbon fabric in epoxy matrix due to the deposition of multi and single walled CNT on fibers [3].

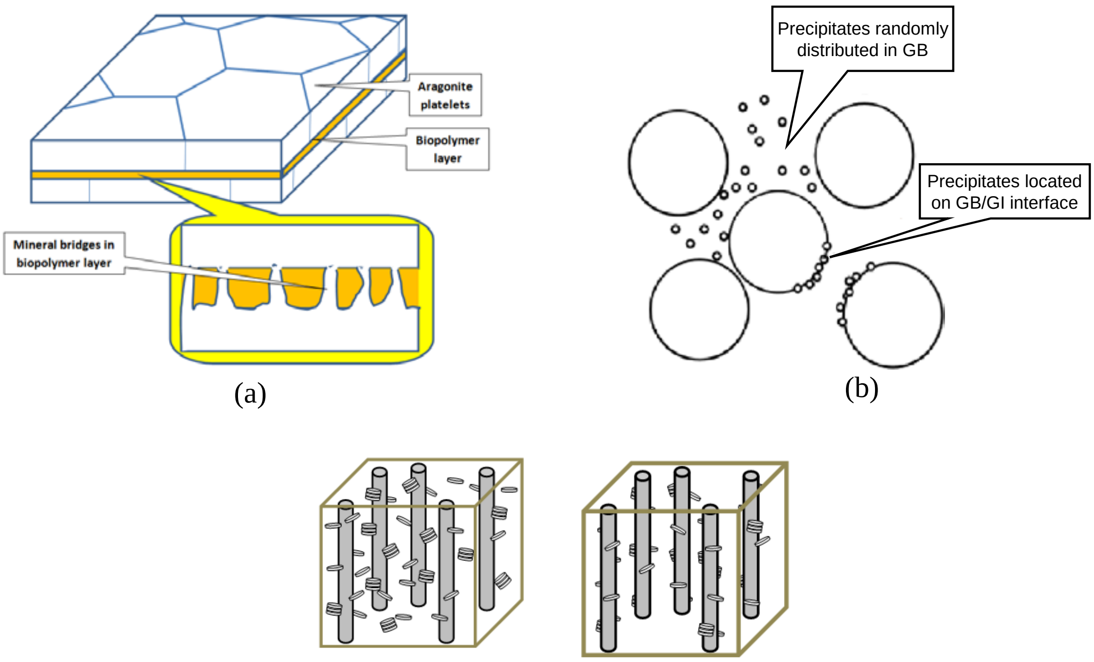
The potential advantages of hierarchical composites over neat composites include the synergy between structural elements at several scale levels, possibility to improve competing properties of materials [4], potential to improve the interface controlled properties, like compression and fatigue strength, by placing nanoparticles on interfaces or fiber sizing, combining the advantages of nanomaterials and composites.

In this paper, the studies of the potential of the improvement of composite service properties based on hierarchical materials design and secondary nanoscale reinforcement (carbone nanotubes, graphene), carried out at the Department of Wind Energy, Technical University of Denmark, are summarized.

2. Nanostructured interfaces as a source of the improvement of composite properties

Figure 1 shows several examples of hierarchical structures of materials with exceptional properties, observed in experiments: nacre structure (brick mortar structure with polymer layers bridged by mineral nanoparticles), ultrafine grained metal (titanium) with atomistic size particles of grain boundaries [7]-[8] and fiber reinforced composites with secondary nanoreinforcement [9]-[11].

So, nacre of mollusks contains 95% of aragonite platelets and only 5% of biopolymer. Thin layers of biopolymer between the platelets can be considered as interfaces in this material [5]. The biopolymer layers represent organic macromolecules, containing polysacharides and protein fibers. Furthermore, the biopolymer thin layers of nacre contain nanopores and also inorganic mineral bridges, linking the aragonite platelets [5]-[6], see Figure 1. Song and Bai [5] evaluated the fracture toughness in the "brick bridge mortar" structure of nacre and showed that the availability of nanostructures in the nacre interfaces (i.e., mineral bridges between aragonite platelets located in the bioolymer layers) is one of the reasons for the high toughness of nacre. The mineral bridges reinforce the weak interface, and control the crack propagation in the interfaces (biopolymer layers). Layers of constrained disturbed polymers surrounding nanoparticles in polymer ensure the drastic enhancement of nanocomposite properties observed in experiments (like 200% increase in stiffness or strength achieved at 0.5% nanoparticle content) [12]. Nanoparticles (nanoclay or carbon nanotubes) located in fiber/matrix interfaces (fiber sizing) of unidirectional composites allow to increase the fatigue lifetime of the composites drastically, as observed experimentally in [10], [11], [14]. One of reasons of extraordinary strength and toughness of nanocrystalline ultrafine grained metals is the high content of grain boundary phases in these materials [15]. Their properties can be further enhanced if the grain boundaries are non-equilibrium, with high density of dislocations and especially with foreign atoms/precipitates [7]. The availability of precipitates strongly delays the damage growth and ensures 83% increase in the critical strains due to the precipitates, and around 300% increase due to the precipitates located in grain boundaries.



(a) (b)

(c)

Figure 1. Examples of materials with nanostructures interfaces and grain boundaries: (a) Nacre structure (brick mortar structure with polymer layers bridged by mineral nanoparticles), (b) ultrafine grained metal (titanium) with atomistic size particles of grain boundaries [6]-[7] (here, GB means "grain boundary" of the metal) and (c) fiber reinforced composites with secondary nanoreinforcement [8]-[10]. Reprinted from [16], [8] and [11] with kind permission of Elsevier

On the basis of generalization of these observations, it was demonstrated in [16], that the purposeful nanostructuring of interfaces and grain boundaries represents an important reserve of the improvement of the materials properties [16]. Since the material deformation is often localized in and around defects (interfaces and grain boundaries), the structuring of these regions (adding specially arranged and oriented nanoreinforcements, or adding nanoscale defects, changing the local properties) allows to control the deformation and fracture behavior of these weak areas, thus, determining the degradation process in the whole material. Quite often, the interphase layers with low stiffness lead to the localization of deformation, while the internal structures of the interphase layers (like mineral bridges in nacre, or nanoplatelets in sizing of fiber reinforced composites) allow to control the deformation, damage initiation and fracture processes locally.

3. Computational modelling of hierarchical composites

In order to analyze the effect of the distribution of secondary nanoparticles in the matrix and in the interface on the damage behaviour of hierarchical composites, a computational multiscale model was developed, which includes the fiber/matrix interaction at the higher scale level (microlevel) and nanoparticles/epoxy matrix interaction on nanolevel. A set of programs for the automatic generation of 3D multiscale models of composites was developed [11]-[17]. The programs generate command files for the commercial FE software ABAQUS. The unit cell structures are divided into two levels. The high and lower level models are linked by submodelling techniques. The macro (upper level) unit cells contain three phases: the matrix, fibers and "third phase" interphase layers (which characterizes the interface roughness, interphases [1], [18]. Both matrix and the interphase layer might contain nanoreinforcements. A number of 3D multiscale unit cell models of nanoparticles (carbon nanotubes, nanosheets) and fiber reinforced composites have been generated and used for the computational testing of structures of composites. Each unit cell model (upper or lower level) has an average of 100…300k elements.Figure 2 shows an example of a unit cell model. In this model, polymer composites with glass fibers (GFRC), carbon fibers (CFRC) and hybrid fibers (HC) are reinforced with carbon nanotubes. The aspect ratio of CNTs was 1000, and they were distributed in the sizing of the fibers.

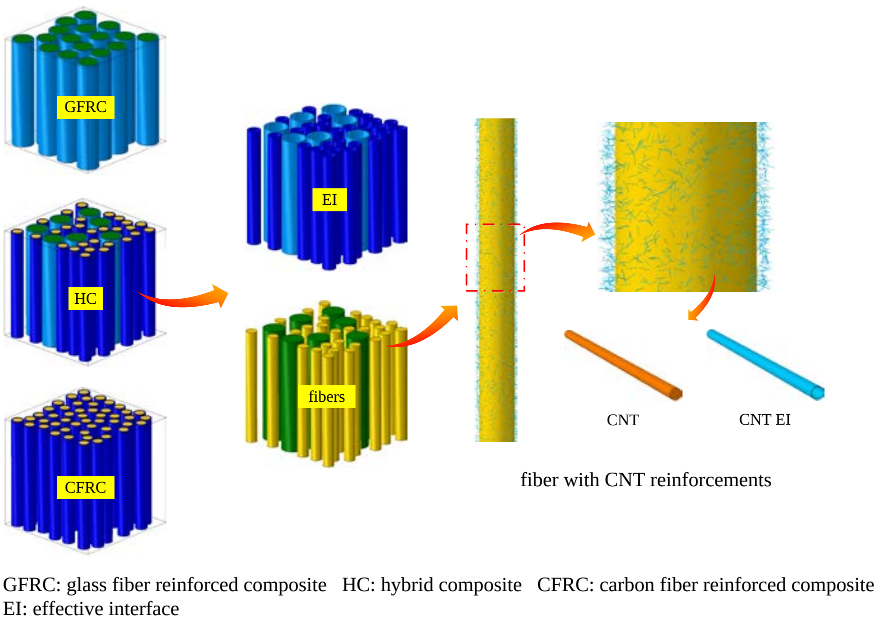


Figure 2. Example of unit cell model of CNT reinforced hybrid composite.Reprinted from [10] with kind permission of Elsevier

The volume fraction of the CNT reinforcement is 0.46%. The model was subject to cyclic compression-tension loading [10]. The crack propagation analysis is carried out in the framework of the linear elastic fracture mechanics (LEFM) approach. The materials are supposed to be elastic. The criteria of damage modelling, materials properties and other details of simulations are described in details in [10].

As a result of simulations, it was shown that the CNT enhances the fatigue performance (stress of the S-N curves corresponding to the same cycles, and lifetime) in all considered composites [10]. For the very low cycle loading, the CNT reinforcement leads to 25%...43% increase in the stress corresponding to a given cycles number (here, taken as 1.72 x 10^7 cycles), while for the millions of cycles, the CNT effect increases the stress by 64…120%. Similarly, the simulations results show that the nanoclay particles located in the matrix or in the fiber sizing, enhance fatigue lifetimes of composites [11].

Figure 3 shows 5 a schema of model of hierarchical fiber composite with nanoclay reinforcements (a) and simulated crack paths in in-between platelets observed in the simulations (aligned and randomly oriented platelets, b and c) [11]. In the simulations, the composites with nanoclay reinforcement achieve the same fatigue life (taken exemplarily at $5.68*10^7$ cycles) as neat composites, while subject to 2…3.5 times higher loadings. As observed in the simulations, composites with the nanoplatelets localized in the fiber/matrix interphase layer (fiber sizing) lead to much higher fatigue lifetime than those with the nanoplatelets in the matrix: 43…49% higher applied stress corresponding to the selected lifetime of $5.68*10^7$ cycles.

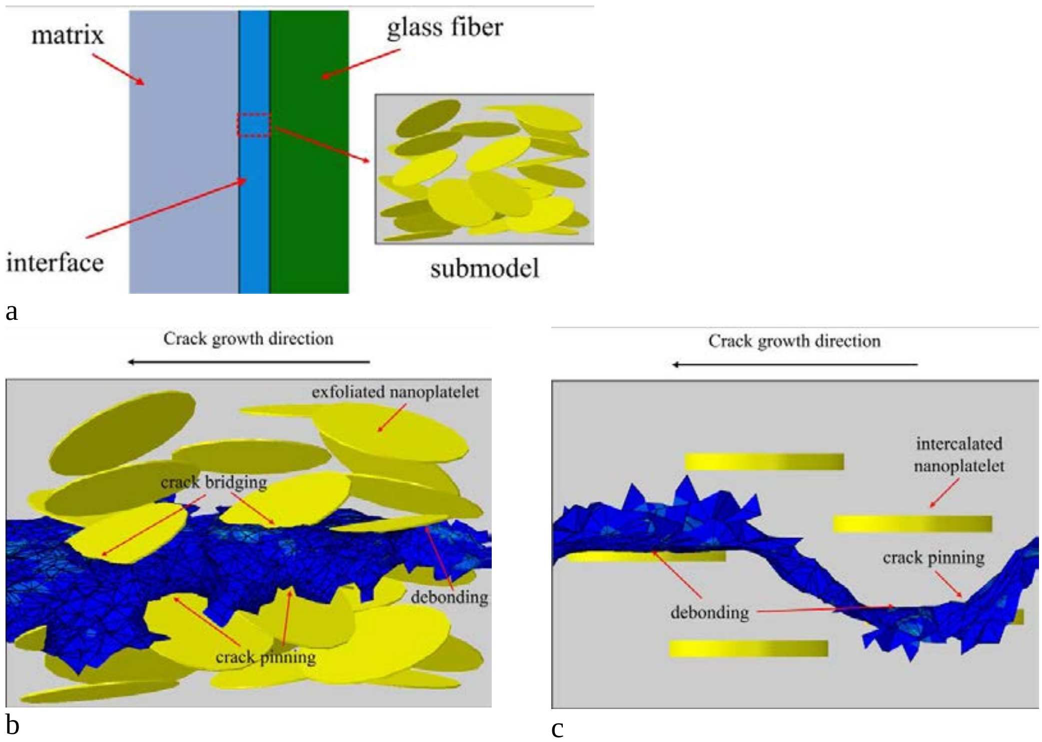
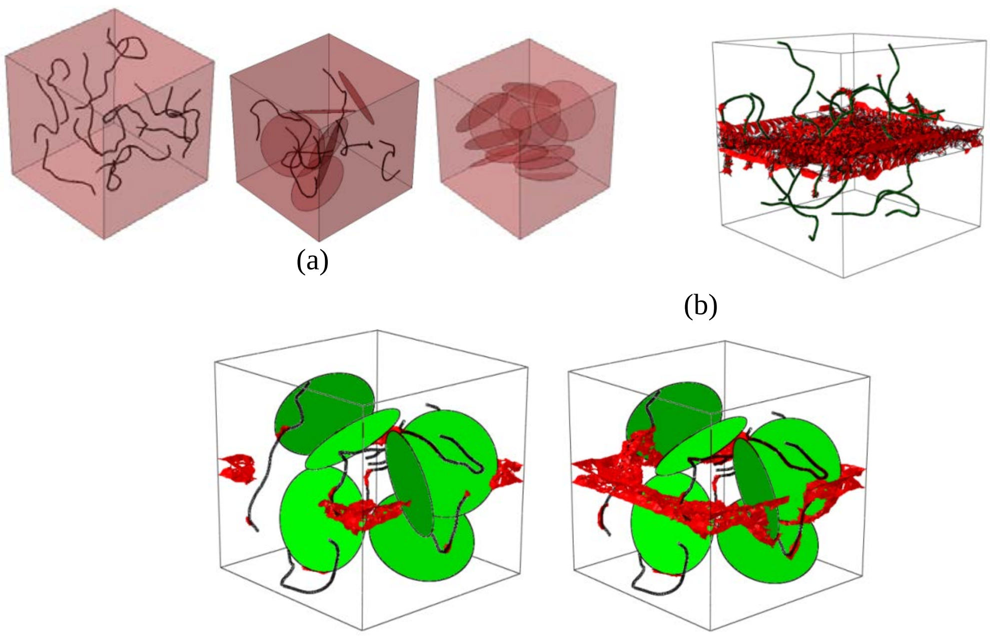


Figure 3. Schema of model of hierarchical fiber composite with nanoclay reinforcements (a) and simulated crack paths in submodels (aligned and randomly oriented platelets, b and c). Reprinted from [[11]] with kind permission of Elsevier

4. Which nanoscale factors control the efficiency of secondary reinforcement?

Nanoscale structure, distribution, shapes and arrangement of secondary nanoreinforcement play a very important role for the optimization of the service properties of hierarchical composites. The effect of the shape, distribution and orientation of nanoparticles (graphene and carbon nanotubes) has been studied in a number of works [13][17]. As demonstrated in the computational studies in [13], the factors influencing the elastic properties and strength of graphene reinforced polymer nanocomposites can be ranked as follows (from stronger to weaker effects): crumpled graphene shape (only for strength: 50% reduction of strength only due to the shape crumpling, but only 10% reduced stiffness) -> graphene sheet misalignment (~50% reduction of stiffness and strength because of misalignment) -> volume content of graphene (50% higher stiffness and 2.5 times higher strength at 4 times higher content of graphene) -> interphase layer strength (7 times higher interphase strength gives only 2.5 times higher composite) and clustering degree (only 25% difference between highly clustered and exfoliated) -> the aspect ratio of sheets (~60% lower strength and 26% higher stiffness due to 20 times higher aspect ratio).

The effect of the shape of carbon nanotube (CNT) reinforcements and hybrid CNT/graphene reinforcements on the strength and damage behavior of nanocomposites has been studied numerically in [17]. Further, the real snake-like shape of carbon nanotubes [19] was taken into account, instead of oversimplified cylindrical models used most often. In order to generate the real snake-like shape of carbon nanotubes (CNT), particles are represented as a chain of hexahedral segments, which is built sequentially, while letting each segment to misalign with respect of the one which precedes it. These segments are joined in the solid modeler module of ABAQUS [17]. The crack growth was modeled using the finite element weakening techniques, implemented in the subroutine User Defined Field. The critical damage value and other simulations details are given in [17].



(a) (b) (c)

Figure 4. Schema of model of hierarchical fiber composite with nanoclay reinforcements (a) and simulated crack paths in submodels (aligned and randomly oriented platelets, b and c). Reprinted from [11] with kind permission of Elsevier

Figure 4a shows the examples of the unit cells with snake-like CNT particles, pure graphene and hybrid CNT/graphene reinforcement. Figure 4bc show the crack path in the unit cell with pure CNT reinforcement and hybrid CNT/graphene reinforcement. As a result of the computational simulation of damage evolution in the unit cells, it was demonstrated that that the synergy effect of hybrid CNT and graphene nanoreinforcement is caused by different interaction of nanoparticles with cracks at different stages of fracture. While graphene particles cause the crack deviation at the early stages of fracture, the CNTs ensure the debonding and fiber bridging mechanisms after the main crack is formed.

In the simulations it was observed that the peak stress for the composite with idealized, cylindrical reinforcement is slightly higher than that for the composite with more realistic, snake-like nanotube reinforcement. Further, it was shown that the real, snake like reinforcements induce higher local stresses and also lead to the earlier failure as compared to the idealized cylinder like models.

5. Conclusions

In this paper, an overview of recent studies of the potential of improving the strength and damage resistance of composites by using hierarchical structure and secondary nanoscale reinforcement, carried out over last years at the Section of Composites and Mechanics of Materials, Department of Wind Energy, Technical University of Denmark, is presented. It is demonstrated that the hierarchical structures of composites represent a promising way for the enhancement of the materials properties. An interesting and promising way to improve the composite strength is nanostructuring of interfaces and other deformable areas, ensuring the control of damage mechanisms. The shapes, orientation and localization of secondary nanoparticle reinforcement play a very important role for the optimization of the materials performances.

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